Glyceryl methacrylate 5919-74-4 | DTXSID7057781

Model Performance

Model Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 42.7 °C

Global applicability domain: Inside

Local applicability domain index: 4.87e-01

Confidence level: 3.82e-01

Nearest Neighbors from the Training Set

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2,2'-Thiobisethanol Measured: -10.2 Predicted: 15.5 Image not found

Triethylene glycol Measured: -7.00 Predicted: 7.03 Image not found

Glyceraldehyde, D-Measured: 145 Predicted: 115

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Diethylene glycol Measured: -10.4 Predicted: -13.2